



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 10:40 AM UTC

PDB ID : 8YMN / pdb_00008ymn
EMDB ID : EMD-39400
Title : OSCA1.1-F516A pre-open 2
Authors : Zhang, M.F.
Deposited on : 2024-03-09
Resolution : 2.50 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

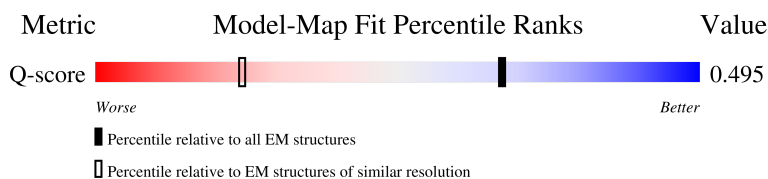
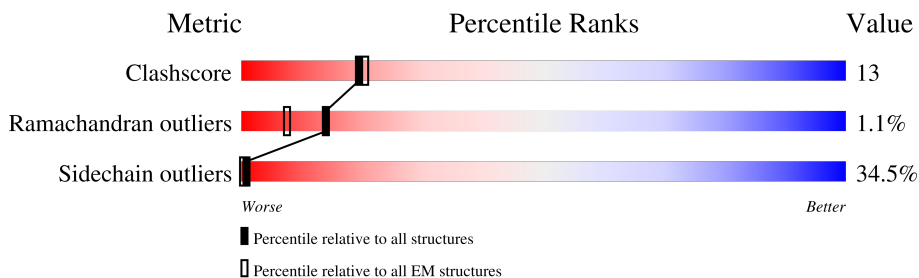
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7115 (2.00 - 3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	772	
1	B	772	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 10728 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

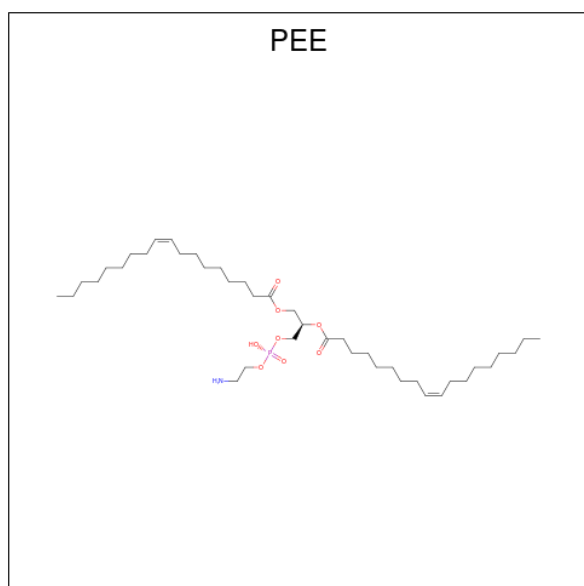
- Molecule 1 is a protein called Protein OSCA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	664	Total	C	N	O	S	0	0
			5346	3526	879	915	26		
1	B	664	Total	C	N	O	S	0	0
			5346	3526	879	915	26		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	516	ALA	PHE	engineered mutation	UNP Q9XEA1
B	516	ALA	PHE	engineered mutation	UNP Q9XEA1

- Molecule 2 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	C	0
			9	9	

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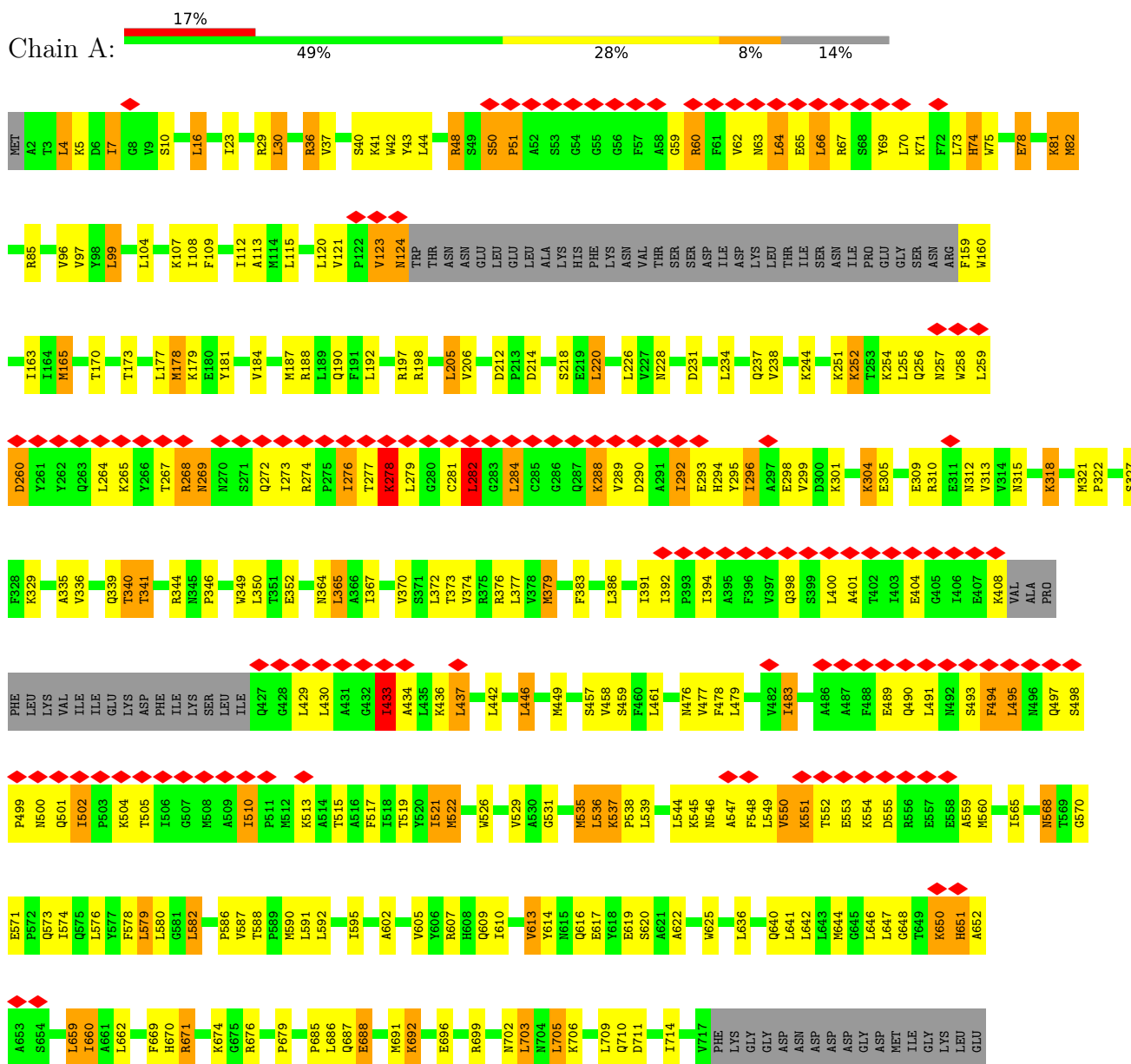
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Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	C	0
			9	9	
2	B	1	Total	C	0
			9	9	
2	B	1	Total	C	0
			9	9	

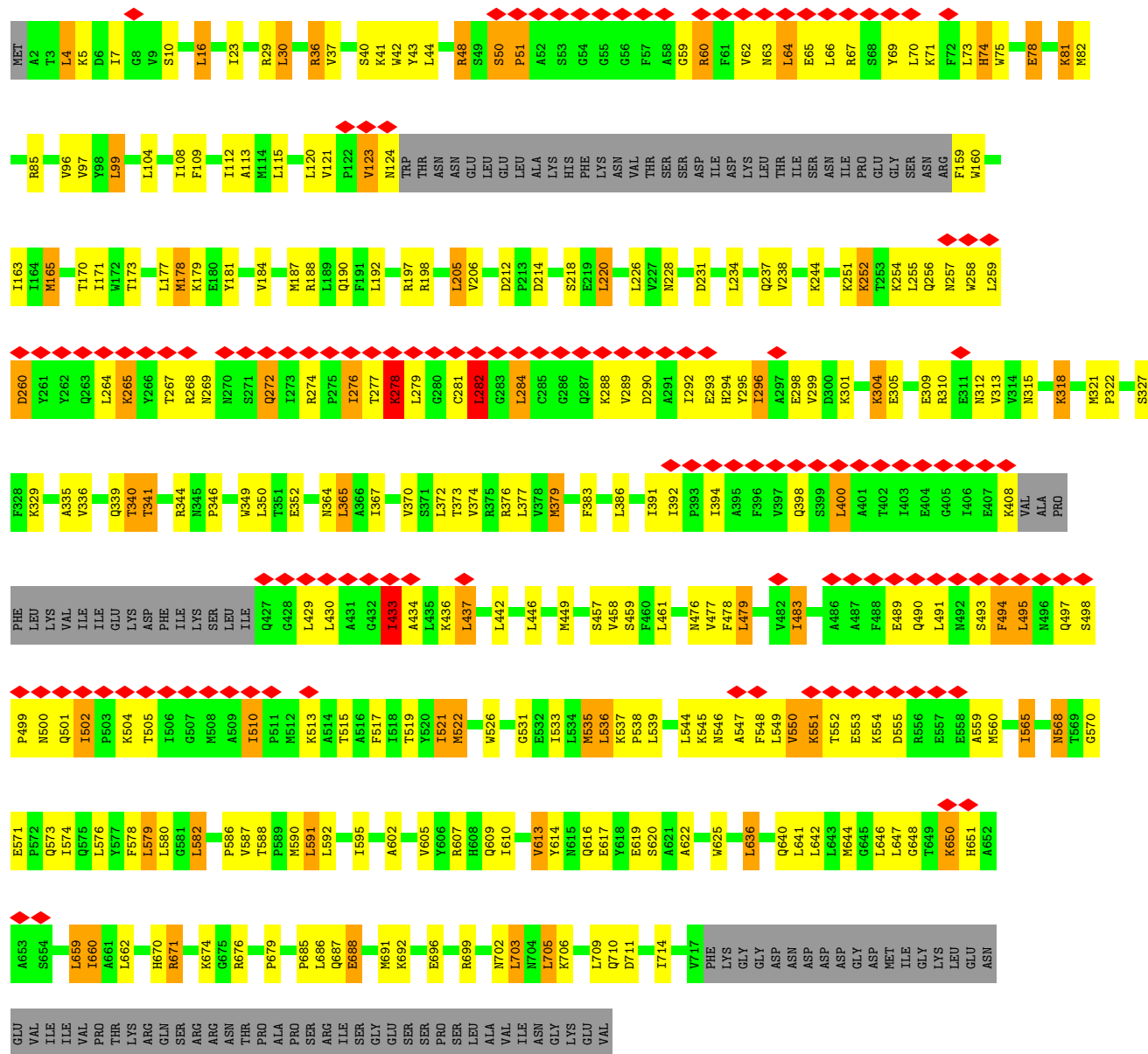
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Protein OSCA1



Chain B:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	83000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.296	Depositor
Minimum map value	-0.187	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	252.0, 252.0, 252.0	wwPDB
Map dimensions	720, 720, 720	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.35, 0.35, 0.35	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.52	0/5493	0.80	14/7469 (0.2%)
1	B	0.52	0/5493	0.80	14/7469 (0.2%)
All	All	0.52	0/10986	0.80	28/14938 (0.2%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	477	VAL	N-CA-C	-6.43	106.53	112.96
1	B	477	VAL	N-CA-C	-6.43	106.53	112.96
1	A	318	LYS	N-CA-C	-6.33	105.49	113.72
1	B	318	LYS	N-CA-C	-6.33	105.49	113.72
1	A	476	ASN	N-CA-C	6.18	120.65	113.18
1	B	476	ASN	N-CA-C	6.18	120.65	113.18
1	A	578	PHE	N-CA-C	-5.95	104.71	111.14
1	B	578	PHE	N-CA-C	-5.95	104.71	111.14
1	A	64	LEU	CB-CA-C	-5.93	109.72	116.54
1	B	64	LEU	CB-CA-C	-5.93	109.72	116.54
1	A	69	TYR	N-CA-C	-5.62	107.07	114.04
1	B	69	TYR	N-CA-C	-5.62	107.07	114.04
1	A	660	ILE	N-CA-C	-5.60	106.86	113.42
1	B	660	ILE	N-CA-C	-5.60	106.86	113.42
1	A	547	ALA	N-CA-C	-5.58	106.83	113.97
1	B	547	ALA	N-CA-C	-5.58	106.83	113.97
1	A	614	TYR	N-CA-C	5.41	118.19	110.24
1	B	614	TYR	N-CA-C	5.41	118.19	110.24
1	A	510	ILE	CA-C-N	-5.28	114.50	120.89
1	A	510	ILE	C-N-CA	-5.28	114.50	120.89
1	B	510	ILE	CA-C-N	-5.28	114.50	120.89
1	B	510	ILE	C-N-CA	-5.28	114.50	120.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	559	ALA	N-CA-C	-5.24	106.75	112.72
1	B	559	ALA	N-CA-C	-5.24	106.75	112.72
1	A	260	ASP	N-CA-C	-5.23	105.66	111.36
1	B	260	ASP	N-CA-C	-5.23	105.66	111.36
1	A	123	VAL	N-CA-C	5.18	111.76	106.21
1	B	123	VAL	N-CA-C	5.18	111.76	106.21

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5346	0	5419	159	0
1	B	5346	0	5419	152	0
2	A	18	0	34	5	0
2	B	18	0	34	5	0
All	All	10728	0	10906	273	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (273) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:ILE:HB	1:A:510:ILE:CG2	1.39	1.51
1:B:483:ILE:HB	1:B:510:ILE:CG2	1.39	1.50
1:B:483:ILE:CB	1:B:510:ILE:CG2	2.09	1.29
1:A:483:ILE:CB	1:A:510:ILE:CG2	2.09	1.29
1:B:255:LEU:CD1	1:B:298:GLU:OE2	1.90	1.20
1:A:255:LEU:CD1	1:A:298:GLU:OE2	1.90	1.19
1:A:686:LEU:HD22	1:B:340:THR:HG21	1.19	1.16
1:B:165:MET:HE1	1:B:586:PRO:HA	1.28	1.14
1:A:340:THR:HG21	1:B:686:LEU:CD2	1.80	1.12
1:A:340:THR:HG21	1:B:686:LEU:HD22	1.19	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:MET:CE	1:A:586:PRO:HA	1.81	1.10
1:A:686:LEU:CD2	1:B:340:THR:HG21	1.80	1.10
1:A:483:ILE:HG12	1:A:510:ILE:HG23	1.27	1.10
1:B:165:MET:CE	1:B:586:PRO:HA	1.81	1.10
1:A:165:MET:HE1	1:A:586:PRO:HA	1.28	1.09
1:B:483:ILE:HG12	1:B:510:ILE:HG23	1.27	1.09
1:A:686:LEU:HD22	1:B:340:THR:CG2	1.85	1.07
1:B:483:ILE:CG1	1:B:510:ILE:CG2	2.32	1.06
1:A:340:THR:CG2	1:B:686:LEU:HD22	1.85	1.05
1:A:483:ILE:CG1	1:A:510:ILE:CG2	2.32	1.05
1:A:483:ILE:CB	1:A:510:ILE:HG22	1.78	1.04
1:A:228:ASN:HD21	1:B:687:GLN:HA	1.22	1.02
1:A:483:ILE:CG1	1:A:510:ILE:HG23	1.88	1.02
1:B:483:ILE:HB	1:B:510:ILE:HG21	1.40	1.02
1:A:687:GLN:HA	1:B:228:ASN:HD21	1.22	1.01
1:B:483:ILE:CB	1:B:510:ILE:HG21	1.89	1.01
1:B:483:ILE:HG12	1:B:510:ILE:CG2	1.91	1.01
1:B:483:ILE:CG1	1:B:510:ILE:HG23	1.88	1.00
1:A:483:ILE:HG12	1:A:510:ILE:CG2	1.91	0.98
1:B:483:ILE:CB	1:B:510:ILE:HG22	1.78	0.97
1:A:483:ILE:CB	1:A:510:ILE:HG21	1.89	0.96
1:A:483:ILE:HB	1:A:510:ILE:HG21	1.40	0.95
1:A:679:PRO:HG2	1:B:346:PRO:HG3	1.48	0.94
1:A:259:LEU:HB2	1:A:294:HIS:H	1.32	0.94
1:A:346:PRO:HG3	1:B:679:PRO:HG2	1.48	0.93
1:A:483:ILE:HB	1:A:510:ILE:HG22	0.93	0.92
1:B:483:ILE:HB	1:B:510:ILE:HG22	0.93	0.92
1:B:259:LEU:HB2	1:B:294:HIS:H	1.32	0.92
1:A:228:ASN:ND2	1:B:687:GLN:HA	1.84	0.91
1:A:687:GLN:HA	1:B:228:ASN:ND2	1.84	0.91
1:B:255:LEU:HD13	1:B:298:GLU:OE2	1.72	0.90
1:A:255:LEU:HD13	1:A:298:GLU:OE2	1.72	0.88
1:B:255:LEU:HD11	1:B:298:GLU:OE2	1.79	0.82
1:A:687:GLN:CA	1:B:228:ASN:HD21	1.92	0.82
1:A:228:ASN:HD21	1:B:687:GLN:CA	1.92	0.82
1:A:255:LEU:HD11	1:A:298:GLU:OE2	1.79	0.79
1:B:531:GLY:HA3	2:B:802:PEE:H74	1.66	0.77
1:A:346:PRO:HG3	1:B:679:PRO:CG	2.16	0.76
1:A:679:PRO:CG	1:B:346:PRO:HG3	2.16	0.76
1:A:531:GLY:HA3	2:A:801:PEE:H74	1.66	0.75
1:A:344:ARG:NH2	1:B:688:GLU:OE1	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:LEU:HD23	2:A:801:PEE:H66	1.69	0.73
1:B:536:LEU:HD23	2:B:802:PEE:H66	1.69	0.73
1:B:165:MET:HE1	1:B:586:PRO:CA	2.16	0.72
1:A:688:GLU:OE1	1:B:344:ARG:NH2	2.21	0.72
1:B:165:MET:HE3	1:B:586:PRO:HA	1.74	0.68
1:A:165:MET:HE3	1:A:586:PRO:HA	1.74	0.68
1:B:536:LEU:HD23	2:B:802:PEE:C40	2.25	0.67
1:A:519:THR:HA	1:A:522:MET:HE2	1.76	0.67
1:A:340:THR:HG21	1:B:686:LEU:HD21	1.76	0.67
1:B:519:THR:HA	1:B:522:MET:HE2	1.76	0.66
1:B:483:ILE:CG2	1:B:510:ILE:HG21	2.25	0.66
1:A:165:MET:HE1	1:A:586:PRO:CA	2.16	0.66
1:A:483:ILE:CG2	1:A:510:ILE:HG21	2.25	0.66
1:A:536:LEU:HD23	2:A:801:PEE:C40	2.25	0.66
1:A:339:GLN:HE21	1:B:341:THR:H	1.44	0.65
1:A:568:ASN:HD22	1:A:568:ASN:H	1.45	0.64
1:A:339:GLN:NE2	1:B:341:THR:H	1.96	0.64
1:A:341:THR:H	1:B:339:GLN:HE21	1.44	0.64
1:A:341:THR:H	1:B:339:GLN:NE2	1.96	0.64
1:B:568:ASN:H	1:B:568:ASN:HD22	1.45	0.64
1:B:255:LEU:HD12	1:B:298:GLU:OE2	1.95	0.62
1:A:686:LEU:HD21	1:B:340:THR:HG21	1.76	0.61
1:A:228:ASN:ND2	1:B:687:GLN:CA	2.59	0.61
1:A:494:PHE:CE2	1:A:495:LEU:HD13	2.36	0.61
1:A:274:ARG:H	1:A:284:LEU:H	1.50	0.59
1:B:494:PHE:CE2	1:B:495:LEU:HD13	2.36	0.59
1:A:255:LEU:HD12	1:A:298:GLU:OE2	1.95	0.58
1:A:687:GLN:CA	1:B:228:ASN:ND2	2.59	0.58
1:B:109:PHE:HA	1:B:112:ILE:HG12	1.86	0.58
1:B:274:ARG:H	1:B:284:LEU:H	1.50	0.57
1:A:670:HIS:HD2	1:A:671:ARG:HH22	1.52	0.57
1:B:670:HIS:HD2	1:B:671:ARG:HH22	1.52	0.57
1:A:109:PHE:HA	1:A:112:ILE:HG12	1.86	0.57
1:B:276:ILE:O	1:B:278:LYS:NZ	2.38	0.57
1:B:59:GLY:HA2	1:B:63:ASN:HD21	1.70	0.56
1:B:212:ASP:HB3	1:B:220:LEU:HD21	1.88	0.56
1:A:276:ILE:O	1:A:278:LYS:NZ	2.38	0.56
1:A:59:GLY:HA2	1:A:63:ASN:HD21	1.70	0.55
1:A:198:ARG:HH12	1:A:619:GLU:HB3	1.71	0.55
1:A:212:ASP:HB3	1:A:220:LEU:HD21	1.88	0.54
1:B:198:ARG:HH12	1:B:619:GLU:HB3	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:494:PHE:HD1	1:B:502:ILE:HG12	1.73	0.54
1:B:670:HIS:CD2	1:B:671:ARG:HH22	2.26	0.54
1:A:494:PHE:HD1	1:A:502:ILE:HG12	1.73	0.54
1:A:165:MET:CE	1:A:586:PRO:CA	2.72	0.53
1:A:670:HIS:CD2	1:A:671:ARG:HH22	2.26	0.53
1:A:36:ARG:HA	1:A:43:TYR:CE2	2.43	0.53
1:A:339:GLN:NE2	1:B:341:THR:HG22	2.24	0.53
1:B:99:LEU:HD21	1:B:607:ARG:HA	1.90	0.53
1:A:99:LEU:HD21	1:A:607:ARG:HA	1.90	0.53
1:B:165:MET:CE	1:B:586:PRO:CA	2.72	0.53
1:A:341:THR:HG22	1:B:339:GLN:NE2	2.24	0.52
1:B:36:ARG:HA	1:B:43:TYR:CE2	2.43	0.52
1:A:42:TRP:HB3	1:A:48:ARG:HB2	1.91	0.52
1:A:602:ALA:HA	1:A:605:VAL:HG22	1.91	0.52
1:B:42:TRP:HB3	1:B:48:ARG:HB2	1.91	0.52
1:B:602:ALA:HA	1:B:605:VAL:HG22	1.91	0.52
1:A:340:THR:OG1	1:B:339:GLN:HG3	2.11	0.51
1:B:458:VAL:HA	1:B:461:LEU:HD12	1.92	0.51
1:B:535:MET:HE3	1:B:538:PRO:HG2	1.93	0.51
1:A:341:THR:CG2	1:B:339:GLN:HE22	2.24	0.51
1:B:379:MET:HE3	1:B:449:MET:HG2	1.93	0.51
1:A:339:GLN:HG3	1:B:340:THR:OG1	2.11	0.51
1:A:379:MET:HE3	1:A:449:MET:HG2	1.93	0.51
1:B:36:ARG:HA	1:B:43:TYR:HE2	1.76	0.50
1:A:458:VAL:HA	1:A:461:LEU:HD12	1.92	0.50
1:A:535:MET:HE3	1:A:538:PRO:HG2	1.93	0.50
1:B:97:VAL:HG21	1:B:622:ALA:HB2	1.94	0.50
1:A:36:ARG:HA	1:A:43:TYR:HE2	1.76	0.50
1:A:339:GLN:HE22	1:B:341:THR:CG2	2.24	0.50
1:A:483:ILE:HG21	1:A:510:ILE:HG21	1.93	0.50
1:B:336:VAL:O	1:B:340:THR:HB	2.12	0.50
1:B:483:ILE:HG21	1:B:510:ILE:HG21	1.93	0.49
1:A:97:VAL:HG21	1:A:622:ALA:HB2	1.94	0.49
1:A:336:VAL:O	1:A:340:THR:HB	2.12	0.49
1:B:609:GLN:HA	1:B:613:VAL:HG23	1.94	0.49
1:A:257:ASN:HA	1:A:260:ASP:HB2	1.95	0.49
1:B:257:ASN:HA	1:B:260:ASP:HB2	1.95	0.49
1:A:228:ASN:HD21	1:B:687:GLN:CB	2.26	0.49
1:A:609:GLN:HA	1:A:613:VAL:HG23	1.94	0.49
1:A:437:LEU:HD12	1:A:437:LEU:HA	1.70	0.48
1:A:170:THR:HG21	1:A:640:GLN:HE21	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ILE:HB	1:A:278:LYS:NZ	2.29	0.48
1:A:36:ARG:HG2	1:A:51:PRO:HG3	1.95	0.48
1:A:687:GLN:CB	1:B:228:ASN:HD21	2.26	0.48
1:A:16:LEU:HD22	1:A:16:LEU:HA	1.73	0.48
1:B:170:THR:HG21	1:B:640:GLN:HE21	1.79	0.48
1:B:276:ILE:HB	1:B:278:LYS:NZ	2.29	0.47
1:A:75:TRP:HH2	1:A:605:VAL:HG12	1.80	0.47
2:B:802:PEE:H75	2:B:802:PEE:H82	1.69	0.47
1:A:124:ASN:HD22	1:A:124:ASN:HA	1.51	0.47
1:A:568:ASN:H	1:A:568:ASN:ND2	2.10	0.47
1:B:550:VAL:HG13	1:B:551:LYS:H	1.80	0.47
1:B:568:ASN:H	1:B:568:ASN:ND2	2.10	0.47
1:A:550:VAL:HG13	1:A:551:LYS:H	1.80	0.46
1:A:4:LEU:H	1:A:4:LEU:HG	1.55	0.46
1:B:36:ARG:HG2	1:B:51:PRO:HG3	1.95	0.46
1:A:341:THR:HG23	1:B:339:GLN:HE22	1.80	0.46
1:B:178:MET:HE3	1:B:178:MET:HB3	1.68	0.46
1:A:50:SER:O	1:A:51:PRO:C	2.58	0.46
1:A:321:MET:HE3	1:A:322:PRO:HD2	1.97	0.46
1:B:321:MET:HE3	1:B:322:PRO:HD2	1.97	0.46
1:A:82:MET:HE3	1:A:82:MET:HB3	1.84	0.46
1:B:75:TRP:HH2	1:B:605:VAL:HG12	1.80	0.46
1:B:674:LYS:HE3	1:B:674:LYS:HB3	1.71	0.46
1:B:50:SER:O	1:B:51:PRO:C	2.58	0.46
1:A:252:LYS:HB3	1:A:252:LYS:HE2	1.58	0.46
1:A:339:GLN:HE22	1:B:341:THR:HG23	1.80	0.46
1:B:479:LEU:H	1:B:479:LEU:HG	1.35	0.46
1:A:60:ARG:H	1:A:60:ARG:HG3	1.53	0.45
1:A:517:PHE:O	1:A:521:ILE:HG12	2.16	0.45
1:A:278:LYS:HZ2	1:A:278:LYS:HG3	1.29	0.45
1:B:165:MET:HE3	1:B:165:MET:HB3	1.30	0.45
1:A:30:LEU:HD12	1:A:30:LEU:HA	1.85	0.45
1:A:78:GLU:HA	1:A:81:LYS:HD2	1.98	0.45
1:A:36:ARG:H	1:A:36:ARG:HG3	1.41	0.45
1:B:517:PHE:O	1:B:521:ILE:HG12	2.16	0.45
1:A:449:MET:HE3	1:A:449:MET:HB3	1.85	0.45
1:A:478:PHE:HD2	1:A:579:LEU:HD13	1.82	0.45
1:A:234:LEU:HD13	1:A:329:LYS:HG2	1.99	0.45
2:A:802:PEE:H67	2:A:802:PEE:H73	1.67	0.45
1:A:205:LEU:HD11	1:A:365:LEU:HD11	1.99	0.45
1:A:537:LYS:HE3	1:A:537:LYS:HB3	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:LYS:HB3	1:B:265:LYS:HE3	1.77	0.44
1:B:536:LEU:HD12	1:B:536:LEU:HA	1.85	0.44
2:B:801:PEE:H73	2:B:801:PEE:H67	1.67	0.44
1:A:674:LYS:HB3	1:A:674:LYS:HE3	1.71	0.44
1:B:78:GLU:HA	1:B:81:LYS:HD2	1.98	0.44
1:A:109:PHE:HE1	1:A:582:LEU:HD13	1.83	0.44
1:B:522:MET:O	1:B:526:TRP:HB2	2.17	0.44
1:A:66:LEU:HD22	1:A:66:LEU:HA	1.82	0.44
1:B:234:LEU:HD13	1:B:329:LYS:HG2	1.99	0.44
1:B:437:LEU:HD12	1:B:437:LEU:HA	1.70	0.44
1:A:685:PRO:HG2	1:A:688:GLU:HB2	2.00	0.44
1:B:565:ILE:H	1:B:565:ILE:HG13	1.50	0.44
1:B:662:LEU:HD12	1:B:662:LEU:HA	1.74	0.44
1:A:433:ILE:HB	1:A:434:ALA:H	1.53	0.44
1:A:522:MET:O	1:A:526:TRP:HB2	2.17	0.44
1:B:99:LEU:HD12	1:B:99:LEU:HA	1.85	0.44
1:B:478:PHE:HD2	1:B:579:LEU:HD13	1.82	0.44
1:A:99:LEU:HD12	1:A:99:LEU:HA	1.85	0.44
1:A:570:GLY:O	1:A:574:ILE:HG13	2.18	0.44
2:A:801:PEE:H75	2:A:801:PEE:H82	1.69	0.44
1:B:109:PHE:HE1	1:B:582:LEU:HD13	1.83	0.44
1:B:685:PRO:HG2	1:B:688:GLU:HB2	2.00	0.44
1:A:383:PHE:HB2	1:A:449:MET:HE1	1.99	0.43
1:B:272:GLN:H	1:B:272:GLN:HG2	1.55	0.43
1:B:495:LEU:HD12	1:B:495:LEU:HA	1.86	0.43
1:A:340:THR:CG2	1:B:686:LEU:CD2	2.65	0.43
1:B:383:PHE:HB2	1:B:449:MET:HE1	1.99	0.43
1:B:205:LEU:HD11	1:B:365:LEU:HD11	1.99	0.43
1:A:288:LYS:H	1:A:288:LYS:HG3	1.55	0.43
1:B:278:LYS:HZ2	1:B:278:LYS:HG3	1.30	0.43
1:B:274:ARG:H	1:B:284:LEU:N	2.17	0.43
1:B:650:LYS:HE2	1:B:650:LYS:HB2	1.37	0.43
1:A:341:THR:N	1:B:339:GLN:HE21	2.15	0.43
1:A:573:GLN:HE21	1:A:573:GLN:HB3	1.59	0.43
1:A:644:MET:HG3	1:A:659:LEU:HB3	2.00	0.43
1:A:107:LYS:HB2	1:A:107:LYS:HE3	1.77	0.43
1:A:304:LYS:HA	1:A:304:LYS:HD3	1.44	0.43
1:B:570:GLY:O	1:B:574:ILE:HG13	2.18	0.43
1:B:644:MET:HG3	1:B:659:LEU:HB3	2.00	0.43
1:A:339:GLN:O	1:B:339:GLN:O	2.36	0.42
1:A:521:ILE:HG12	1:A:521:ILE:H	1.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:LEU:HD12	1:A:662:LEU:HA	1.74	0.42
1:B:252:LYS:HB3	1:B:252:LYS:HE2	1.58	0.42
1:A:650:LYS:HE2	1:A:650:LYS:HB2	1.37	0.42
1:A:703:LEU:HD13	1:A:705:LEU:HD22	2.01	0.42
1:B:591:LEU:HD13	1:B:591:LEU:HA	1.84	0.42
1:A:165:MET:HE3	1:A:165:MET:HB3	1.30	0.42
1:B:206:VAL:HG21	1:B:349:TRP:HE3	1.84	0.42
1:A:401:ALA:HA	1:A:404:GLU:HG3	2.02	0.42
1:A:364:ASN:HA	1:A:367:ILE:HG13	2.02	0.42
1:B:60:ARG:H	1:B:60:ARG:HG3	1.53	0.42
1:A:97:VAL:HG21	1:A:622:ALA:CB	2.49	0.42
1:A:292:ILE:H	1:A:292:ILE:HG12	1.69	0.42
1:B:97:VAL:HG21	1:B:622:ALA:CB	2.49	0.42
1:B:533:ILE:HD12	1:B:533:ILE:HA	1.96	0.42
1:A:108:ILE:HD13	1:A:173:THR:HG23	2.02	0.42
1:A:339:GLN:NE2	1:B:341:THR:CG2	2.82	0.41
1:B:16:LEU:HA	1:B:16:LEU:HD22	1.73	0.41
1:B:281:CYS:O	1:B:282:LEU:C	2.63	0.41
1:A:268:ARG:HB2	1:A:269:ASN:H	1.56	0.41
1:B:36:ARG:H	1:B:36:ARG:HG3	1.41	0.41
1:A:7:ILE:HA	1:A:7:ILE:HD13	1.72	0.41
1:A:120:LEU:HD11	1:A:165:MET:HE1	2.03	0.41
1:A:206:VAL:HG21	1:A:349:TRP:HE3	1.84	0.41
1:A:281:CYS:O	1:A:282:LEU:C	2.63	0.41
1:A:522:MET:HE2	1:A:522:MET:HB2	1.85	0.41
1:A:692:LYS:HZ2	1:A:692:LYS:HG2	1.78	0.41
1:A:651:HIS:HB3	1:A:652:ALA:H	1.57	0.41
1:B:108:ILE:HD13	1:B:173:THR:HG23	2.02	0.41
1:B:703:LEU:HD13	1:B:705:LEU:HD22	2.01	0.41
1:B:400:LEU:HD13	1:B:400:LEU:HA	1.87	0.41
1:B:335:ALA:O	1:B:339:GLN:HG2	2.21	0.41
1:B:365:LEU:HD13	1:B:365:LEU:HA	1.88	0.41
1:A:178:MET:HE3	1:A:178:MET:HB3	1.68	0.41
1:A:341:THR:CG2	1:B:339:GLN:NE2	2.82	0.41
1:B:4:LEU:H	1:B:4:LEU:HG	1.55	0.41
1:B:70:LEU:O	1:B:74:HIS:HB2	2.21	0.41
1:B:304:LYS:HD3	1:B:304:LYS:HA	1.44	0.41
1:B:30:LEU:HD12	1:B:30:LEU:HA	1.85	0.41
1:B:120:LEU:HD11	1:B:165:MET:HE1	2.03	0.41
1:A:70:LEU:O	1:A:74:HIS:HB2	2.21	0.40
1:A:113:ALA:HA	1:A:592:LEU:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ILE:HA	1:A:284:LEU:HD13	2.03	0.40
1:A:483:ILE:HG12	1:A:510:ILE:HG21	1.92	0.40
1:B:304:LYS:HZ2	1:B:304:LYS:HG2	1.78	0.40
1:A:184:VAL:HA	1:A:187:MET:HE3	2.02	0.40
1:A:529:VAL:HB	1:A:605:VAL:HG21	2.03	0.40
1:B:113:ALA:HA	1:B:592:LEU:HD13	2.03	0.40
1:A:339:GLN:HE21	1:B:341:THR:N	2.15	0.40
1:B:184:VAL:HA	1:B:187:MET:HE3	2.02	0.40
1:B:364:ASN:HA	1:B:367:ILE:HG13	2.02	0.40
1:B:433:ILE:HB	1:B:434:ALA:H	1.53	0.40
1:B:573:GLN:HE21	1:B:573:GLN:HB3	1.59	0.40
1:A:178:MET:HB2	1:A:669:PHE:HE1	1.87	0.40
1:A:335:ALA:O	1:A:339:GLN:HG2	2.21	0.40
1:A:446:LEU:HD12	1:A:446:LEU:HA	1.95	0.40
1:A:495:LEU:HD12	1:A:495:LEU:HA	1.86	0.40
1:B:171:ILE:HD13	1:B:171:ILE:HA	1.92	0.40
1:B:636:LEU:HD12	1:B:636:LEU:HA	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	658/772 (85%)	578 (88%)	73 (11%)	7 (1%)	11	22
1	B	658/772 (85%)	578 (88%)	73 (11%)	7 (1%)	11	22
All	All	1316/1544 (85%)	1156 (88%)	146 (11%)	14 (1%)	14	22

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	PRO

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Mol	Chain	Res	Type
1	B	51	PRO
1	A	296	ILE
1	A	433	ILE
1	B	296	ILE
1	B	433	ILE
1	A	499	PRO
1	B	499	PRO
1	A	278	LYS
1	A	282	LEU
1	B	278	LYS
1	B	282	LEU
1	A	648	GLY
1	B	648	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	568/665 (85%)	372 (66%)	196 (34%)	0	0
1	B	568/665 (85%)	372 (66%)	196 (34%)	0	0
All	All	1136/1330 (85%)	744 (66%)	392 (34%)	1	0

All (392) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	5	LYS
1	A	7	ILE
1	A	10	SER
1	A	16	LEU
1	A	23	ILE
1	A	29	ARG
1	A	30	LEU
1	A	36	ARG
1	A	37	VAL

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Mol	Chain	Res	Type
1	A	40	SER
1	A	41	LYS
1	A	44	LEU
1	A	48	ARG
1	A	50	SER
1	A	60	ARG
1	A	62	VAL
1	A	64	LEU
1	A	65	GLU
1	A	66	LEU
1	A	67	ARG
1	A	71	LYS
1	A	73	LEU
1	A	74	HIS
1	A	78	GLU
1	A	81	LYS
1	A	82	MET
1	A	85	ARG
1	A	96	VAL
1	A	99	LEU
1	A	104	LEU
1	A	115	LEU
1	A	121	VAL
1	A	123	VAL
1	A	124	ASN
1	A	159	PHE
1	A	160	TRP
1	A	163	ILE
1	A	165	MET
1	A	177	LEU
1	A	178	MET
1	A	179	LYS
1	A	181	TYR
1	A	188	ARG
1	A	190	GLN
1	A	192	LEU
1	A	197	ARG
1	A	205	LEU
1	A	214	ASP
1	A	218	SER
1	A	220	LEU
1	A	226	LEU

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Mol	Chain	Res	Type
1	A	231	ASP
1	A	237	GLN
1	A	238	VAL
1	A	244	LYS
1	A	251	LYS
1	A	252	LYS
1	A	254	LYS
1	A	256	GLN
1	A	258	TRP
1	A	264	LEU
1	A	265	LYS
1	A	267	THR
1	A	268	ARG
1	A	269	ASN
1	A	272	GLN
1	A	276	ILE
1	A	277	THR
1	A	278	LYS
1	A	279	LEU
1	A	282	LEU
1	A	284	LEU
1	A	288	LYS
1	A	289	VAL
1	A	290	ASP
1	A	292	ILE
1	A	293	GLU
1	A	295	TYR
1	A	296	ILE
1	A	299	VAL
1	A	301	LYS
1	A	304	LYS
1	A	305	GLU
1	A	309	GLU
1	A	310	ARG
1	A	312	ASN
1	A	313	VAL
1	A	315	ASN
1	A	318	LYS
1	A	327	SER
1	A	340	THR
1	A	341	THR
1	A	350	LEU

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Mol	Chain	Res	Type
1	A	352	GLU
1	A	365	LEU
1	A	370	VAL
1	A	372	LEU
1	A	373	THR
1	A	374	VAL
1	A	376	ARG
1	A	377	LEU
1	A	379	MET
1	A	386	LEU
1	A	391	ILE
1	A	392	ILE
1	A	394	ILE
1	A	398	GLN
1	A	400	LEU
1	A	408	LYS
1	A	429	LEU
1	A	430	LEU
1	A	433	ILE
1	A	436	LYS
1	A	437	LEU
1	A	442	LEU
1	A	446	LEU
1	A	457	SER
1	A	459	SER
1	A	479	LEU
1	A	483	ILE
1	A	489	GLU
1	A	490	GLN
1	A	491	LEU
1	A	493	SER
1	A	494	PHE
1	A	495	LEU
1	A	497	GLN
1	A	498	SER
1	A	500	ASN
1	A	501	GLN
1	A	502	ILE
1	A	504	LYS
1	A	505	THR
1	A	513	LYS
1	A	515	THR

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Mol	Chain	Res	Type
1	A	521	ILE
1	A	522	MET
1	A	535	MET
1	A	536	LEU
1	A	537	LYS
1	A	539	LEU
1	A	544	LEU
1	A	545	LYS
1	A	546	ASN
1	A	548	PHE
1	A	549	LEU
1	A	550	VAL
1	A	551	LYS
1	A	552	THR
1	A	553	GLU
1	A	554	LYS
1	A	555	ASP
1	A	560	MET
1	A	565	ILE
1	A	568	ASN
1	A	571	GLU
1	A	576	LEU
1	A	579	LEU
1	A	580	LEU
1	A	582	LEU
1	A	587	VAL
1	A	588	THR
1	A	590	MET
1	A	591	LEU
1	A	595	ILE
1	A	610	ILE
1	A	613	VAL
1	A	616	GLN
1	A	617	GLU
1	A	620	SER
1	A	625	TRP
1	A	636	LEU
1	A	641	LEU
1	A	642	LEU
1	A	646	LEU
1	A	647	LEU
1	A	650	LYS

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Mol	Chain	Res	Type
1	A	651	HIS
1	A	659	LEU
1	A	660	ILE
1	A	671	ARG
1	A	676	ARG
1	A	688	GLU
1	A	691	MET
1	A	692	LYS
1	A	696	GLU
1	A	699	ARG
1	A	702	ASN
1	A	703	LEU
1	A	705	LEU
1	A	706	LYS
1	A	709	LEU
1	A	710	GLN
1	A	711	ASP
1	A	714	ILE
1	B	4	LEU
1	B	5	LYS
1	B	7	ILE
1	B	10	SER
1	B	16	LEU
1	B	23	ILE
1	B	29	ARG
1	B	30	LEU
1	B	36	ARG
1	B	37	VAL
1	B	40	SER
1	B	41	LYS
1	B	44	LEU
1	B	48	ARG
1	B	50	SER
1	B	60	ARG
1	B	62	VAL
1	B	64	LEU
1	B	65	GLU
1	B	66	LEU
1	B	67	ARG
1	B	71	LYS
1	B	73	LEU
1	B	74	HIS

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Mol	Chain	Res	Type
1	B	78	GLU
1	B	81	LYS
1	B	82	MET
1	B	85	ARG
1	B	96	VAL
1	B	99	LEU
1	B	104	LEU
1	B	115	LEU
1	B	121	VAL
1	B	123	VAL
1	B	124	ASN
1	B	159	PHE
1	B	160	TRP
1	B	163	ILE
1	B	165	MET
1	B	177	LEU
1	B	178	MET
1	B	179	LYS
1	B	181	TYR
1	B	188	ARG
1	B	190	GLN
1	B	192	LEU
1	B	197	ARG
1	B	205	LEU
1	B	214	ASP
1	B	218	SER
1	B	220	LEU
1	B	226	LEU
1	B	231	ASP
1	B	237	GLN
1	B	238	VAL
1	B	244	LYS
1	B	251	LYS
1	B	252	LYS
1	B	254	LYS
1	B	256	GLN
1	B	258	TRP
1	B	264	LEU
1	B	265	LYS
1	B	267	THR
1	B	268	ARG
1	B	269	ASN

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Mol	Chain	Res	Type
1	B	272	GLN
1	B	276	ILE
1	B	277	THR
1	B	278	LYS
1	B	279	LEU
1	B	282	LEU
1	B	284	LEU
1	B	288	LYS
1	B	289	VAL
1	B	290	ASP
1	B	292	ILE
1	B	293	GLU
1	B	295	TYR
1	B	296	ILE
1	B	299	VAL
1	B	301	LYS
1	B	304	LYS
1	B	305	GLU
1	B	309	GLU
1	B	310	ARG
1	B	312	ASN
1	B	313	VAL
1	B	315	ASN
1	B	318	LYS
1	B	327	SER
1	B	340	THR
1	B	341	THR
1	B	350	LEU
1	B	352	GLU
1	B	365	LEU
1	B	370	VAL
1	B	372	LEU
1	B	373	THR
1	B	374	VAL
1	B	376	ARG
1	B	377	LEU
1	B	379	MET
1	B	386	LEU
1	B	391	ILE
1	B	392	ILE
1	B	394	ILE
1	B	398	GLN

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Mol	Chain	Res	Type
1	B	400	LEU
1	B	408	LYS
1	B	429	LEU
1	B	430	LEU
1	B	433	ILE
1	B	436	LYS
1	B	437	LEU
1	B	442	LEU
1	B	446	LEU
1	B	457	SER
1	B	459	SER
1	B	479	LEU
1	B	483	ILE
1	B	489	GLU
1	B	490	GLN
1	B	491	LEU
1	B	493	SER
1	B	494	PHE
1	B	495	LEU
1	B	497	GLN
1	B	498	SER
1	B	500	ASN
1	B	501	GLN
1	B	502	ILE
1	B	504	LYS
1	B	505	THR
1	B	513	LYS
1	B	515	THR
1	B	521	ILE
1	B	522	MET
1	B	535	MET
1	B	536	LEU
1	B	537	LYS
1	B	539	LEU
1	B	544	LEU
1	B	545	LYS
1	B	546	ASN
1	B	548	PHE
1	B	549	LEU
1	B	550	VAL
1	B	551	LYS
1	B	552	THR

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Mol	Chain	Res	Type
1	B	553	GLU
1	B	554	LYS
1	B	555	ASP
1	B	560	MET
1	B	565	ILE
1	B	568	ASN
1	B	571	GLU
1	B	576	LEU
1	B	579	LEU
1	B	580	LEU
1	B	582	LEU
1	B	587	VAL
1	B	588	THR
1	B	590	MET
1	B	591	LEU
1	B	595	ILE
1	B	610	ILE
1	B	613	VAL
1	B	616	GLN
1	B	617	GLU
1	B	620	SER
1	B	625	TRP
1	B	636	LEU
1	B	641	LEU
1	B	642	LEU
1	B	646	LEU
1	B	647	LEU
1	B	650	LYS
1	B	651	HIS
1	B	659	LEU
1	B	660	ILE
1	B	671	ARG
1	B	676	ARG
1	B	688	GLU
1	B	691	MET
1	B	692	LYS
1	B	696	GLU
1	B	699	ARG
1	B	702	ASN
1	B	703	LEU
1	B	705	LEU
1	B	706	LYS

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Mol	Chain	Res	Type
1	B	709	LEU
1	B	710	GLN
1	B	711	ASP
1	B	714	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	90	HIS
1	A	124	ASN
1	A	190	GLN
1	A	228	ASN
1	A	241	ASN
1	A	256	GLN
1	A	257	ASN
1	A	312	ASN
1	A	339	GLN
1	A	398	GLN
1	A	500	ASN
1	A	501	GLN
1	A	568	ASN
1	A	573	GLN
1	A	575	GLN
1	A	609	GLN
1	A	616	GLN
1	A	629	HIS
1	A	670	HIS
1	A	687	GLN
1	B	14	ASN
1	B	63	ASN
1	B	90	HIS
1	B	124	ASN
1	B	190	GLN
1	B	228	ASN
1	B	241	ASN
1	B	312	ASN
1	B	339	GLN
1	B	398	GLN
1	B	500	ASN
1	B	501	GLN
1	B	568	ASN

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Mol	Chain	Res	Type
1	B	573	GLN
1	B	575	GLN
1	B	609	GLN
1	B	616	GLN
1	B	629	HIS
1	B	670	HIS
1	B	687	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PEE	A	801	-	8,8,50	0.22	0	7,7,55	0.53	0
2	PEE	B	802	-	8,8,50	0.22	0	7,7,55	0.53	0
2	PEE	A	802	-	8,8,50	0.23	0	7,7,55	0.56	0
2	PEE	B	801	-	8,8,50	0.23	0	7,7,55	0.56	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEE	A	801	-	-	5/6/6/54	-
2	PEE	B	802	-	-	5/6/6/54	-
2	PEE	A	802	-	-	3/6/6/54	-
2	PEE	B	801	-	-	3/6/6/54	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	PEE	C42-C43-C44-C45
2	A	802	PEE	C40-C41-C42-C43
2	B	801	PEE	C40-C41-C42-C43
2	B	802	PEE	C42-C43-C44-C45
2	A	802	PEE	C42-C43-C44-C45
2	B	801	PEE	C42-C43-C44-C45
2	A	801	PEE	C40-C41-C42-C43
2	B	802	PEE	C40-C41-C42-C43
2	A	801	PEE	C44-C45-C46-C47
2	B	802	PEE	C44-C45-C46-C47
2	A	802	PEE	C43-C44-C45-C46
2	B	801	PEE	C43-C44-C45-C46
2	A	801	PEE	C41-C42-C43-C44
2	B	802	PEE	C41-C42-C43-C44
2	A	801	PEE	C43-C44-C45-C46
2	B	802	PEE	C43-C44-C45-C46

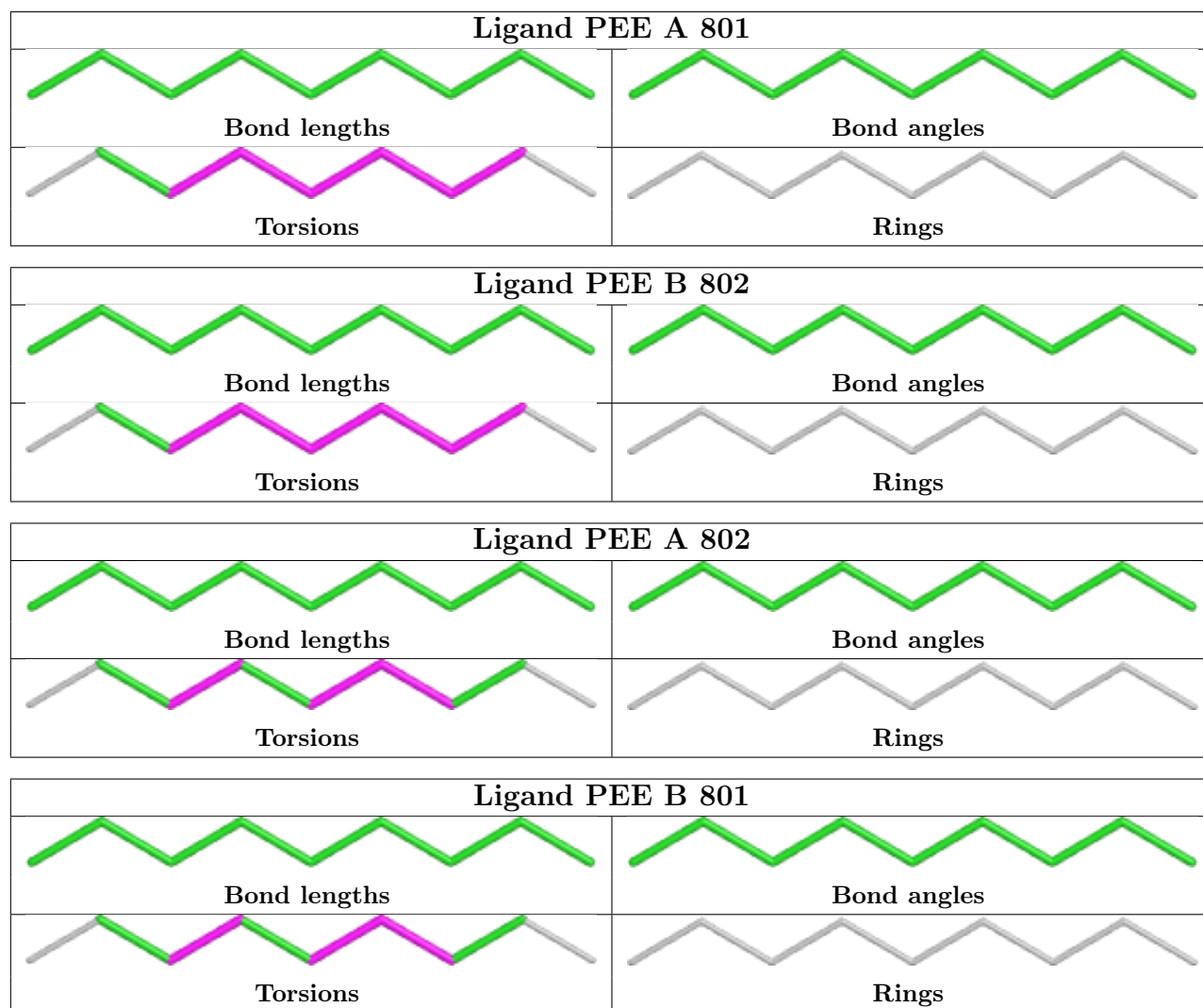
There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	PEE	4	0
2	B	802	PEE	4	0
2	A	802	PEE	1	0
2	B	801	PEE	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

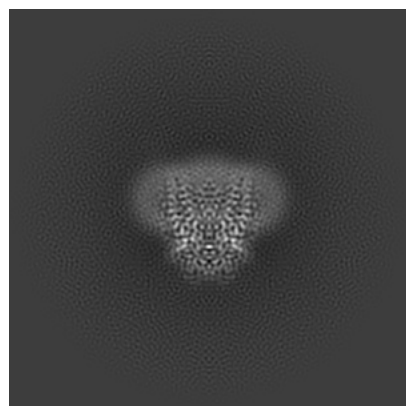
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39400. These allow visual inspection of the internal detail of the map and identification of artifacts.

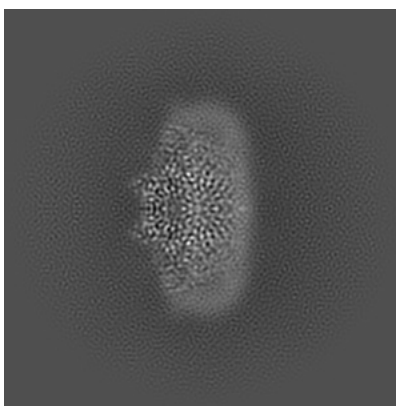
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

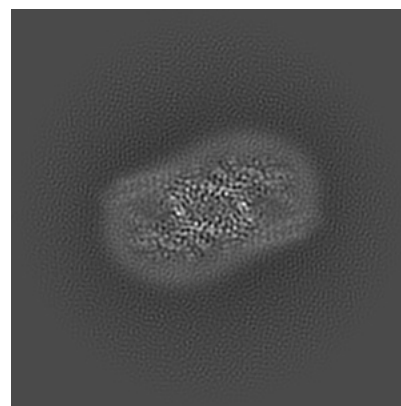
6.1.1 Primary map



X

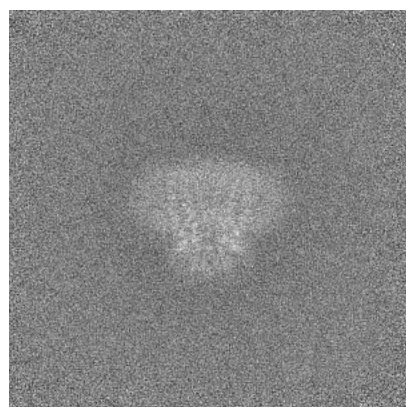


Y

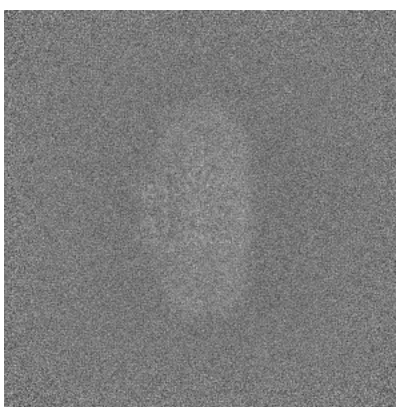


Z

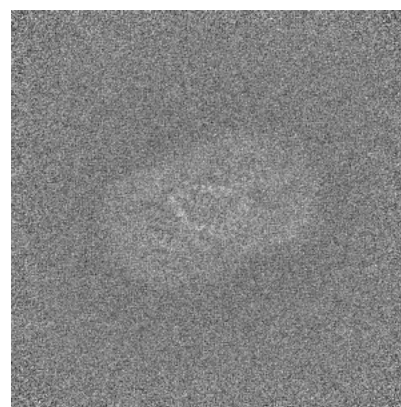
6.1.2 Raw map



X



Y

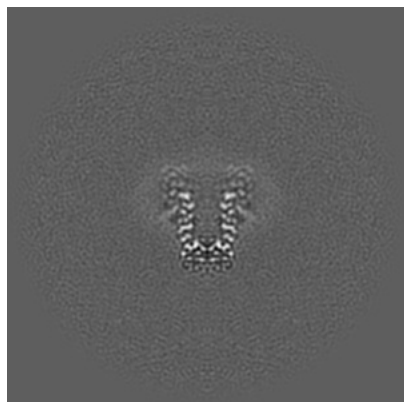


Z

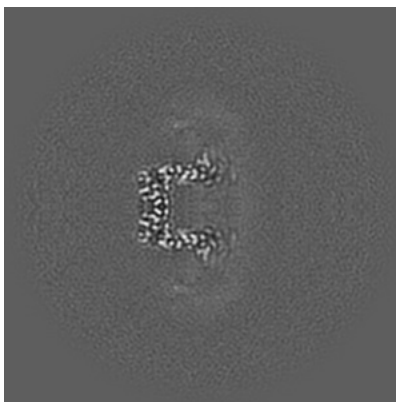
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

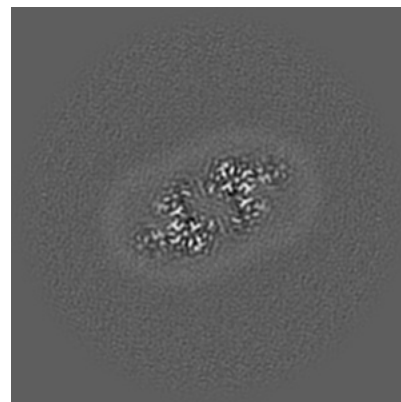
6.2.1 Primary map



X Index: 360

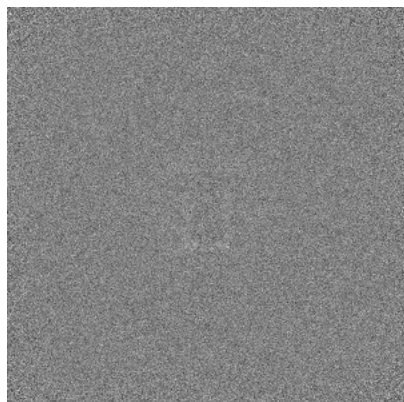


Y Index: 360

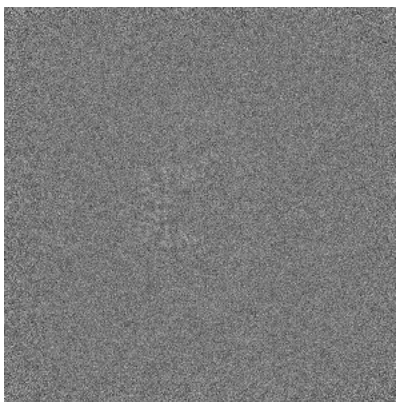


Z Index: 360

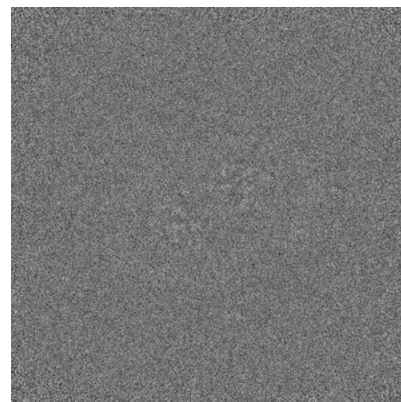
6.2.2 Raw map



X Index: 360



Y Index: 360

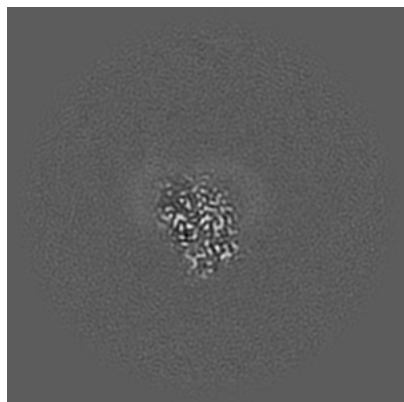


Z Index: 360

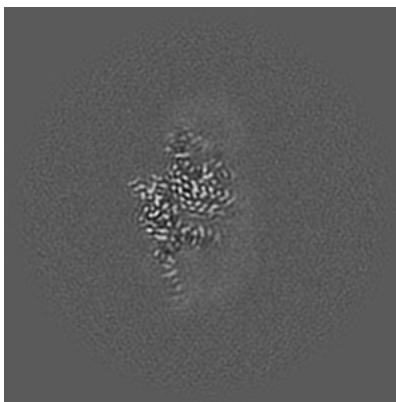
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

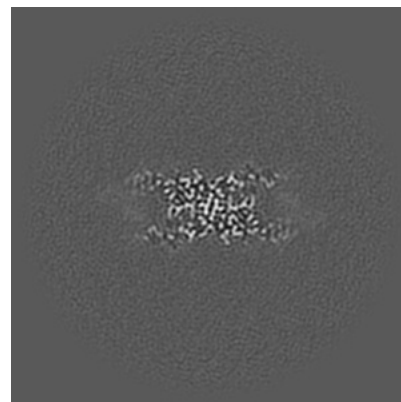
6.3.1 Primary map



X Index: 307

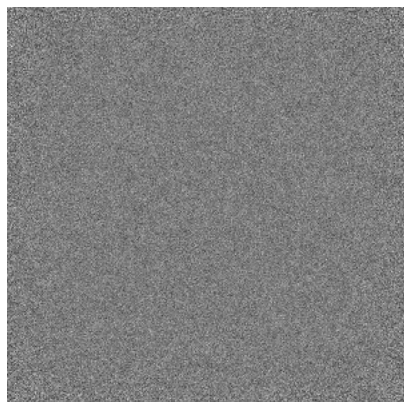


Y Index: 395

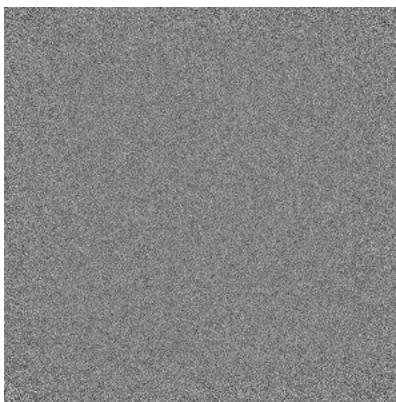


Z Index: 291

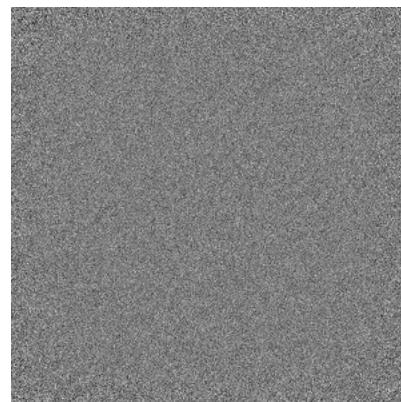
6.3.2 Raw map



X Index: 0



Y Index: 0

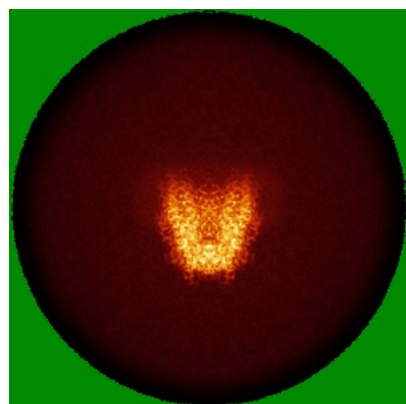


Z Index: 0

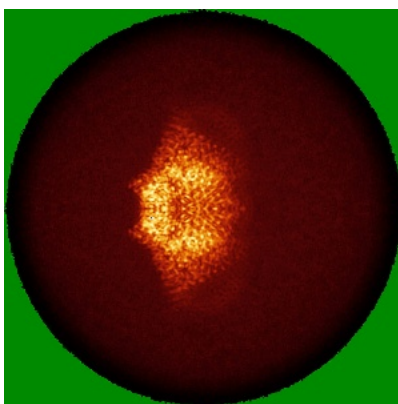
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

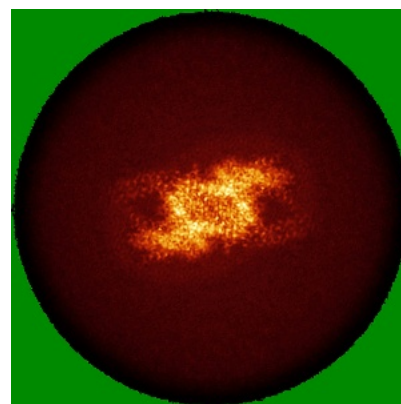
6.4.1 Primary map



X

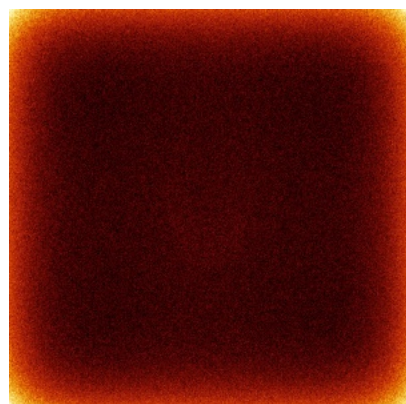


Y

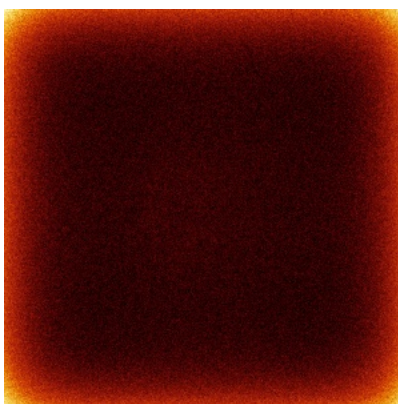


Z

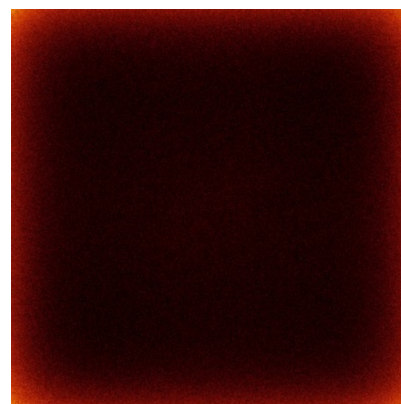
6.4.2 Raw map



X



Y

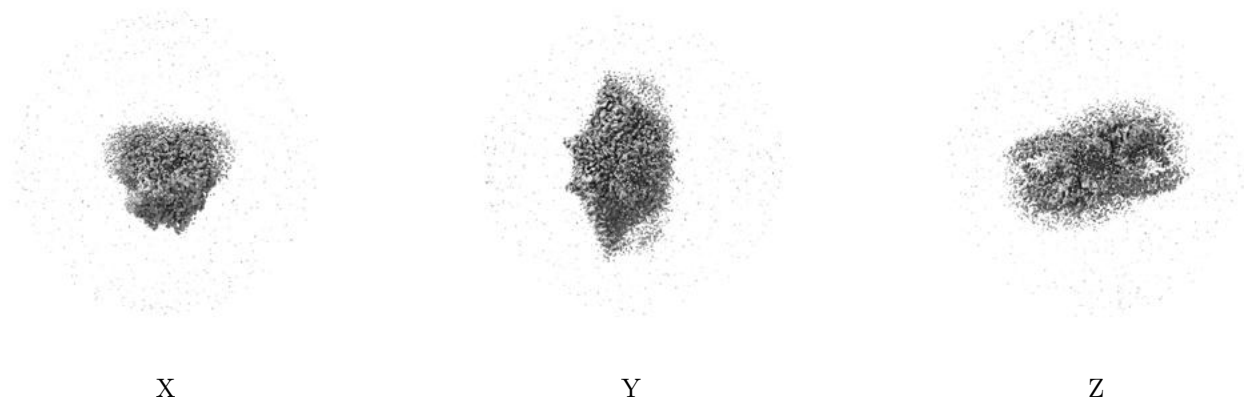


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

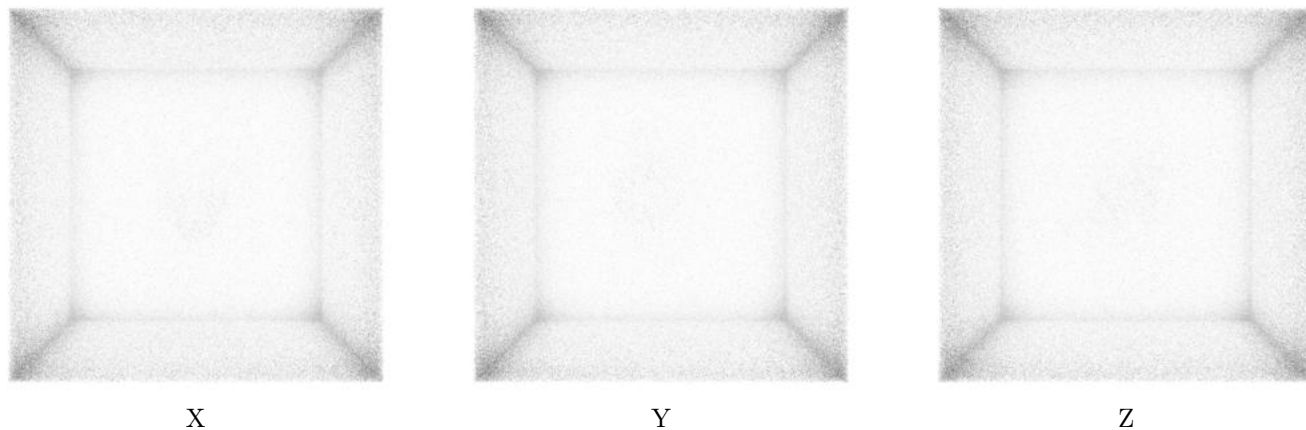
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

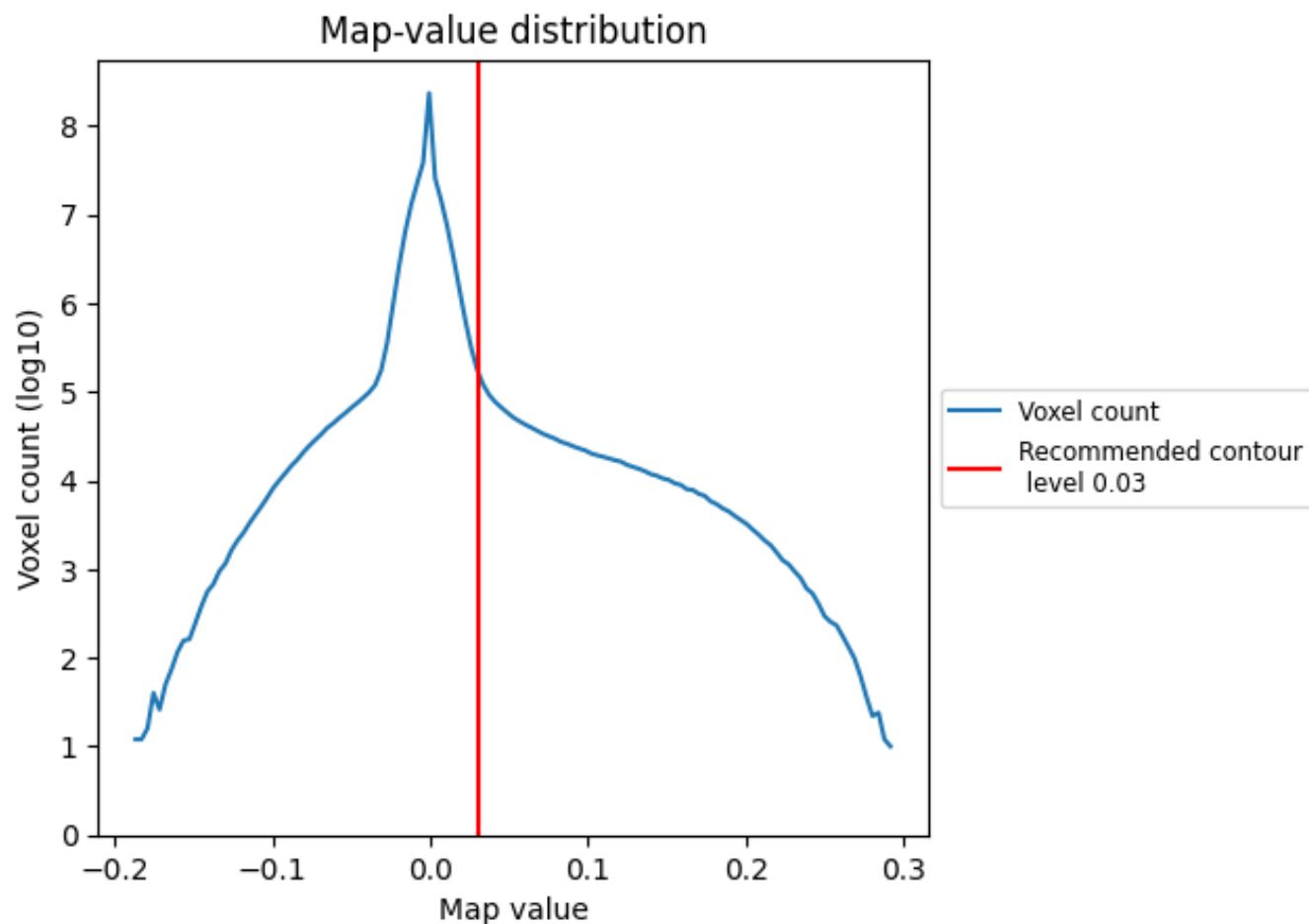
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

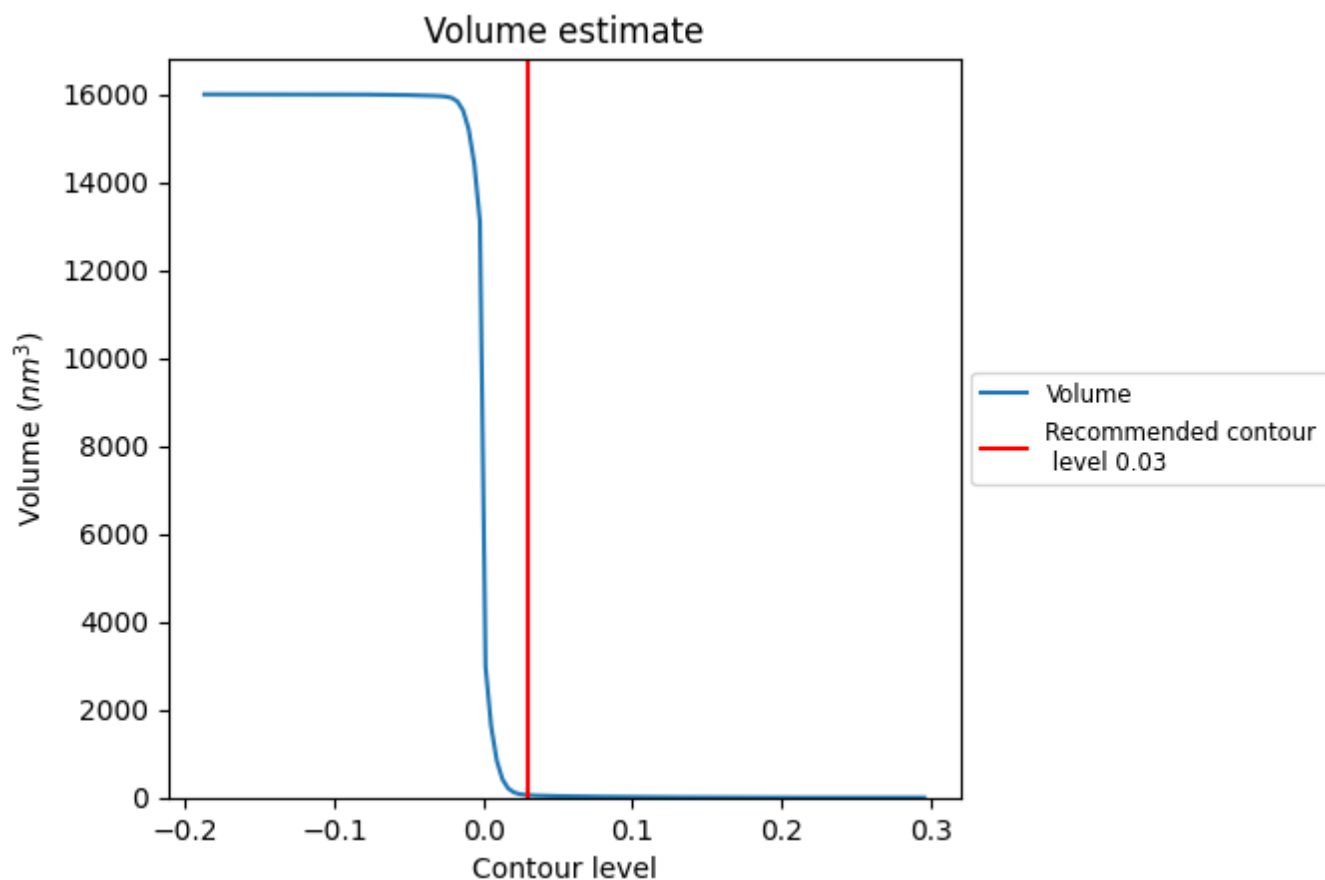
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

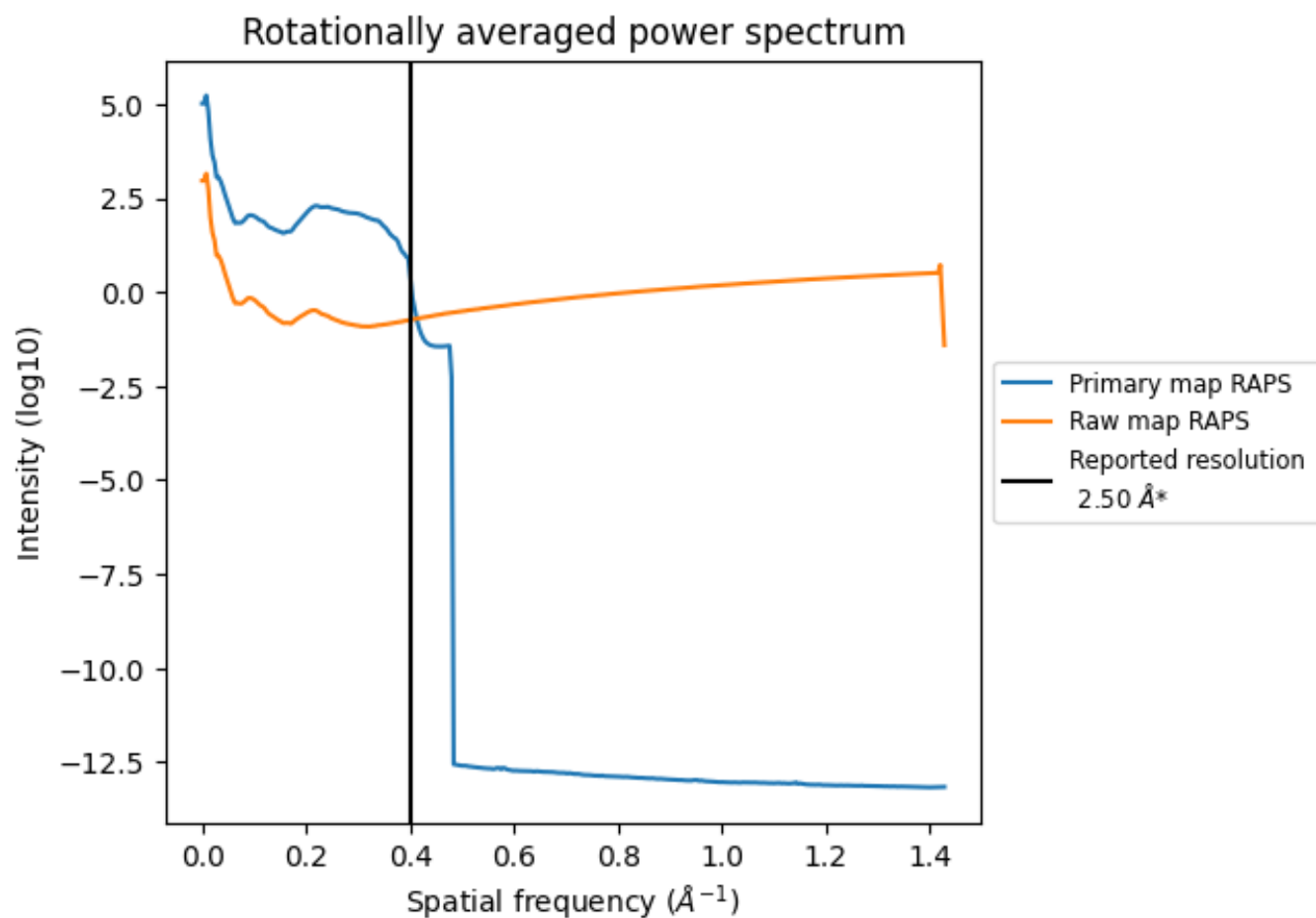
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 57 nm^3 ; this corresponds to an approximate mass of 51 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

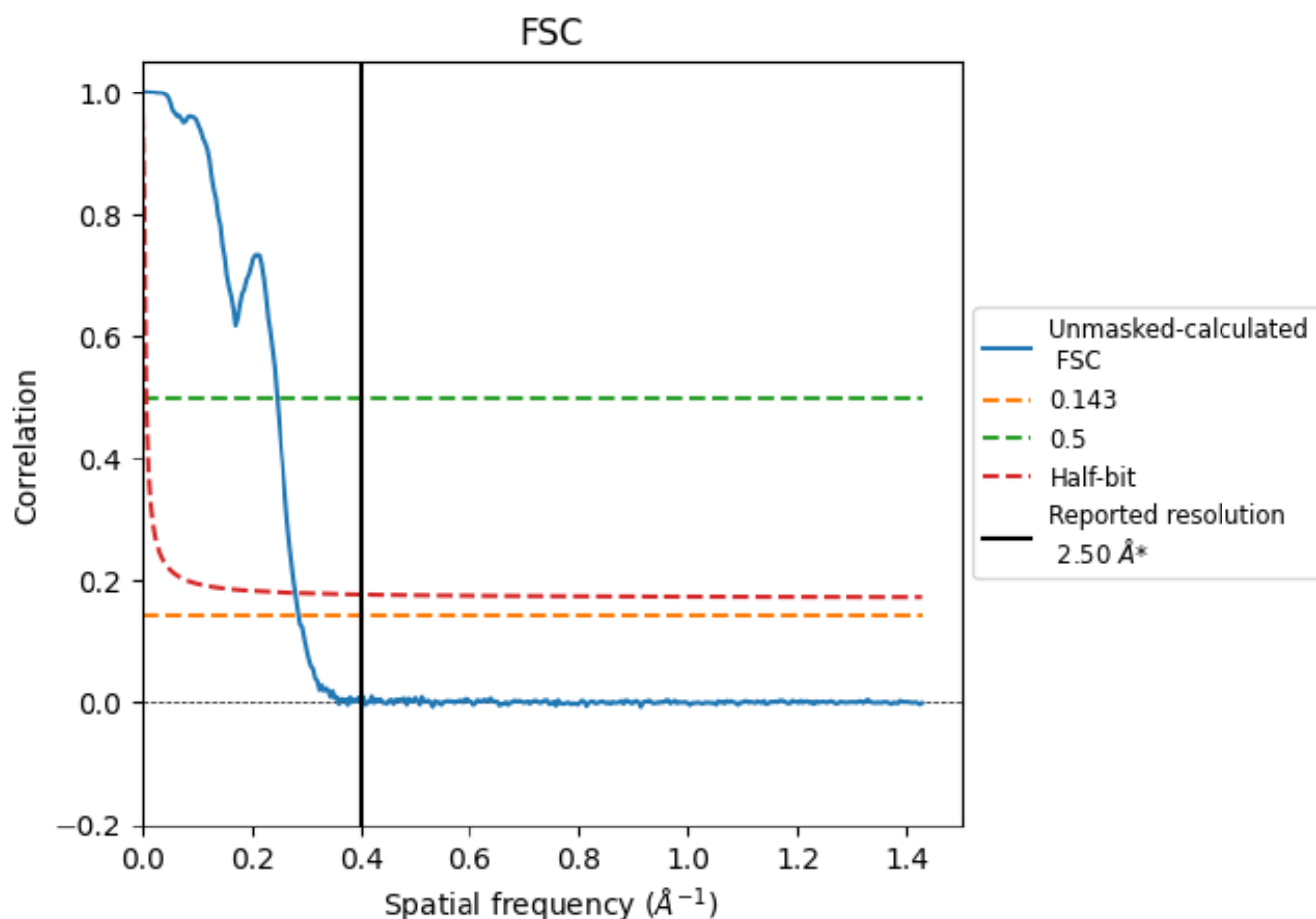


*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

8.2 Resolution estimates [i](#)

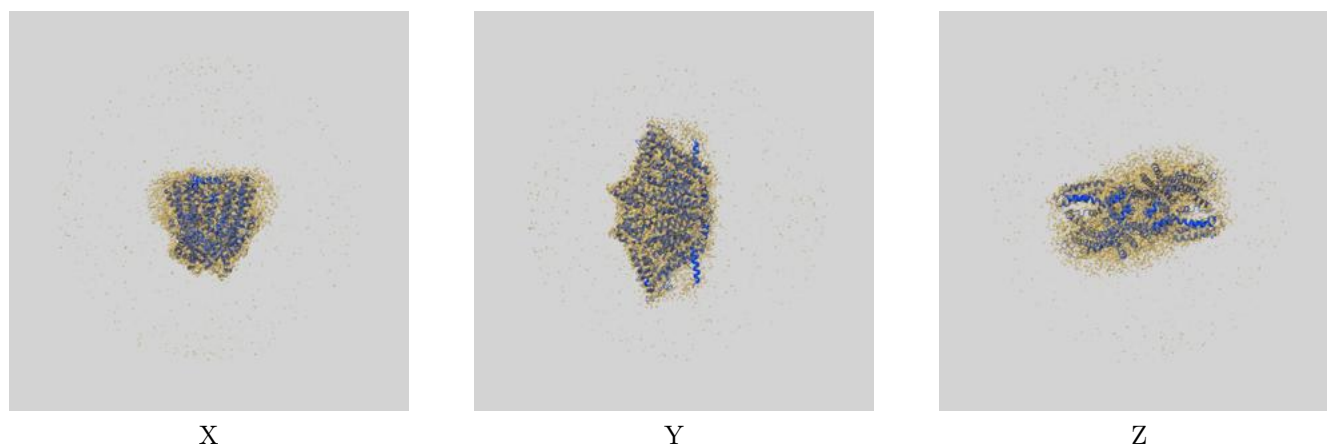
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.48	4.05	3.56

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.48 differs from the reported value 2.5 by more than 10 %

9 Map-model fit [i](#)

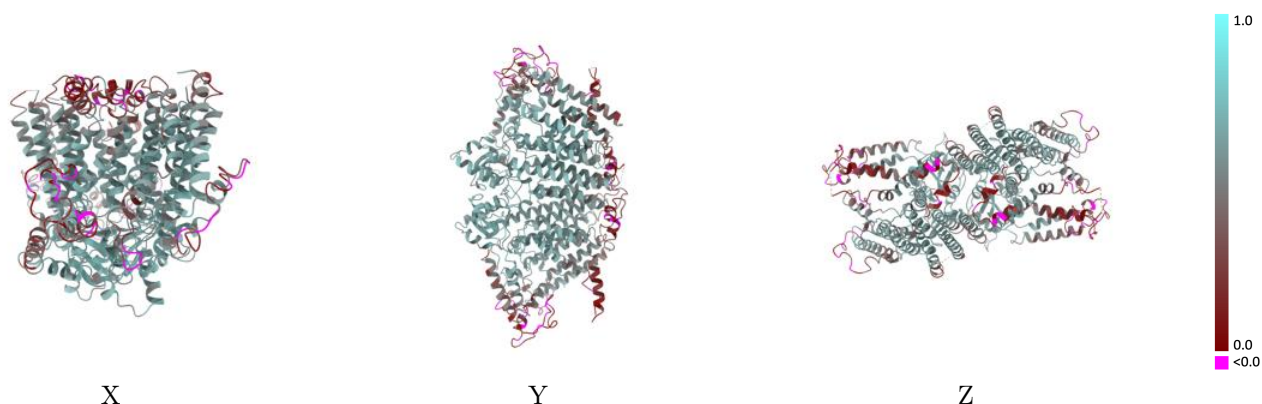
This section contains information regarding the fit between EMDB map EMD-39400 and PDB model 8YMN. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)

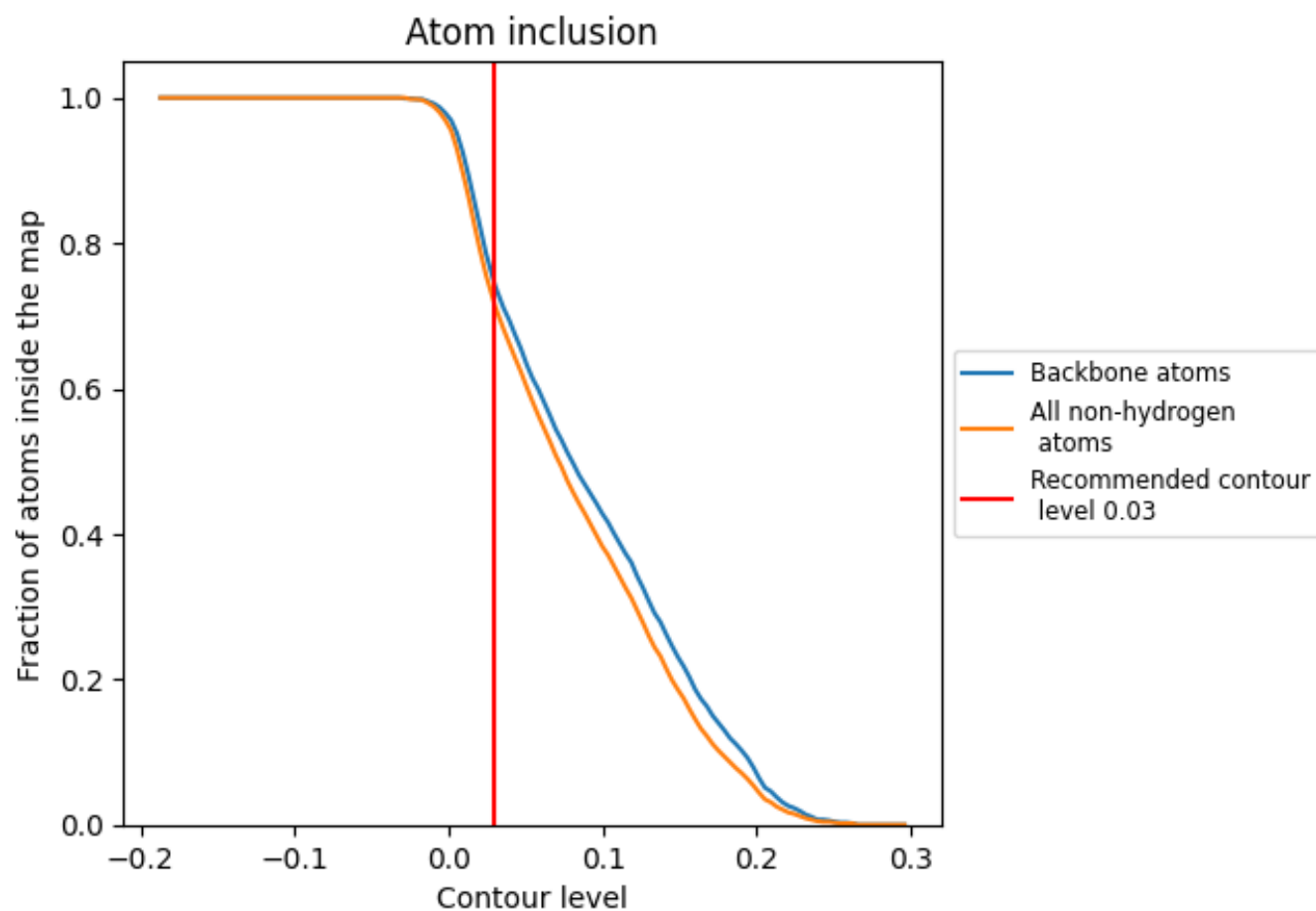


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7140	0.4950
A	0.7140	0.4950
B	0.7140	0.4950

